MC simulations of i-TED 4π & background rejection studies

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Outline

- Introduction to i-TED and motivation

- MC simulation of i-TED: capture and background events
  - i-TED Response to (n,g) and background
  - Imaging of (n,g) and background

- Background rejection based on MC simulations
  - Analytical imaging cuts: the $\lambda$ parameter
  - $(n,g)$/background gain: i-TED vs C6D6
  - ML-based vs analytical background rejection

- ML-based background rejection with i-TED 5.3 data

- Summary
Motivation

- **i-TED Concept:** Combine TED & Compton imaging to reduce extrinsic neutron background

- **Plans for final i-TED-4pi**
  - Under development but not yet commissioned @ n_TOF → no experimental data of final detector
  - Commissioning and Se-79\(\text{n},\text{g}\) measurement in 2021/22
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- **Plans for final i-TED-4pi**
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  - Commissioning and Se-79(n,g) measurement in 2021/22

- **Goal MC simulations:**
  - Optimization of crystal thickness, S-A distance,..
  - Counting rate estimates for Se-79(n,g)
  - Optimization of imaging and background rejection
  - Study of impact of experimental effects (resolution, backscattering, summing,...)
  - Understand results i-TED 5.3 commissioning @ n_TOF and i-TED5 @ IFIC-Lab
**i-TED Concept:** Combine TED & Compton imaging to reduce extrinsic neutron background

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**Goal MC simulations:**
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- **Optimization of imaging and background rejection**
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MC simulations of (n,g) and background events
MC simulations for capture/background discrimination

- CAPTURE:
  - CAPTUGEN Au-197(n,g)

- EXTRINSIC BACKGROUND
  - Experimental data
    - i-TED 5.3 Prototype (2018)
    - (DETAILS IN BACK-UP)

Neutron induced background

Capture event
MC i-TED: Response(n,g) & background

i-TED-5 MC response to (n,g) and background: Singles & coincidences

CAPTURE: Au-197(n,g) (Captugen)  BACKGROUND: Exp. i-TED 5.3 @ EAR1

Absorber more affected by extrinsic background from walls + it shields the scatterer

Coincidences (A & S) reduce more strongly the background →

→ Improved capture/background ratio before imaging
MC i-TED: imaging \((n,g)\) & background

**CAPTURE:** Reconstructed emission point for \((n,g)\) events in the sample

**BACKGROUND:** Reconstructed emission point for background from the walls

A LARGE FRACTION OF CAPTURE SELECTED

MOST OF THE BACKGROUND REJECTED

i-TED IMAGING OPTIMIZATION: Keep \((n,g)\) efficiency high + Maximum \((n,g)/\text{background}\) gain factor
Background rejection based on MC: Imaging and ML algorithms
Imaging cuts using i-TED MC

- Background rejection with imaging cuts: the $\lambda$ parameter

**Low $\lambda$ values:** $\gamma$-rays fulfill the intersection condition between the compton cone and the sample

$\lambda$ distribution for capture and background (MC)

\[
\lambda = \left( n_x a_x + n_y a_y + n_z a_z \right)^2 - \left( 1 + \frac{511}{E_1 + E_2} - \frac{511}{E_2} \right)^2 \left( a_x^2 + a_y^2 + a_z^2 \right)
\]
Imaging cuts using i-TED MC

- Background rejection with imaging cuts: the $\lambda$ parameter

**Low $\lambda$ values:** $\gamma$-rays fulfill the intersection condition between the Compton cone and the sample

$\lambda$ distribution for capture and background (MC)

![Graph showing $\lambda$ distribution for capture and background.]

**$\lambda$ IMAGING CUT**

Difference between $(n,g)$ and background at Low $\lambda$

Clear background rejection with $\lambda<500-1000$
(n,g)/background: i-TED vs C6D6

MC Results of (n,g)/background: i-TED gain with respect to C6D6

i-TED (n,g)/background gain vs. C6D6:

A) Coincidences crystals: Factor 1.5 – 3 (*)

A) Imaging: Cuts in λ parameter

Best gain factors (n, γ)/bckg ratio wrt to C6D6

Values with no imaging cut

TOTAL (n,g)/background gain with IMAGING

i-TED gain factor x 4 - 10

with respect to a C6D6 @ 10 cm

(depending of the sample - i-TED distance)

Cost of THE IMAGING CUTS

(n,g) efficiency reduced to a 20-40%

(for reasonable lambda cuts λ<500-1000)

(*) DETAILS IN BACK-UP
Background rejection based on MC: ML algorithms vs analytic
ML-based (n,g)/bckg discrimination in a nutshell

- i-TED MC EVENTS: E1, E2, p1, p2, (t2-t1)
- ½ CAPTURE
- ½ BACKGROUND

TRAIN ML-ALGORITHM
XGBoost BINARY CLASSIFIER
(70-80% MC events)

TEST THE ML-ALGORITHM
(Remaining 20-30% MC events)
ML-based (n,g)/bckg discrimination

- ML-based capture/background discrimination in a nutshell

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RESULT: CONFUSION MATRIX

FOMs

(n,g) efficiency = True positive

(n,g)/background gain factor = True positive/False Negative

RESULT WITH IDEAL CRT (MC TIME)
ML-based \((n,g)/bckg\) discrimination

- **ML-based capture/background discrimination in a nutshell**

  i-TED MC EVENTS: \(E_1, E_2, p_1, p_2, (t_2-t_1)\)

  \[\frac{1}{2} \text{ CAPTURE} \rightarrow \frac{1}{2} \text{ BACKGROUND}\]

  **TRAIN ML-ALGORITHM**
  - XGBoost BINARY CLASSIFIER
  - (70-80% MC events)

  **TEST THE ML-ALGORITHM**
  - (Remaining 20-30 % MC events)

**RESULT: CONFUSION MATRIX**

- **FOMs**
  - \((n,g)\) efficiency = True positive
  - \((n,g)/\)background gain factor = True positive/False Negative

**RESULT WITH IDEAL CRT (MC TIME)**

Very promising results

**NEXT:** compare to imaging cuts
ML-algorithms vs imaging cut ($\lambda$)

**CAPTURE/BACKGROUND GAIN FACTOR:**

ML (DOTTED) vs $\lambda$ Cut (SOLID)

- ML (XGB) max: 2.8
- ML (XGB) min: 1.7

**FOM#1:**

\[(n,g)/\text{background gain factor} \sim \lambda \text{ Cut} < 300-500\]

(*) Details in the back-up
ML-algorithms vs imaging cut ($\lambda$)

**CAPTURE/BACKGROUND GAIN FACTOR:**
- ML (DOTTED) vs $\lambda$ Cut (SOLID)

**FOM #1:**
- \((n,g)/\text{background gain factor}\)
- ML (n,g)/bckg gain factor $\sim \lambda$ Cut $<300-500$

**CAPTURE EFFICIENCY:**
- ML (DOTTED) vs $\lambda$ Cut (SOLID)

**FOM #2:**
- \((n,g)\) efficiency
- Same \((n,g)/\text{background gain factor}\)
- Efficiency ML is $x$ 2-3 LARGER
Background rejection studies based on i-TED 5.3 data
Results ML classifier: Au-197(n,g)

- ML (n,g)/background (n,g)/bckg classifier: results for Au-197(n,g)

1) Capture efficiency (4.9 eV res)
   - ML (XGB): 80%
   - Analytical $\lambda < 1000$: 34%

2) Peak-to-valley gain factor
   - ML (XGB): 1.24
   - Imaging $\lambda < 1000$: 1.14

Au-197: ML provides high (n,g) eff. but background is already low $\rightarrow$ Fe-56 better to check (n,g)/background gain
Results ML classifier: Fe-56(n,g)

- ML (n,g)/background (n,g)/bckg classifier: results for Fe-56(n,g)

**ML (XGB) training: Exp. Data i-TED prototype (2018)**
Fe-56 (1.15 keV) (capture) + Carbon (background)

1) Capture efficiency (1.15 keV res)
   - **ML (XGB)**: 80%
   - Imaging $\lambda<1000$: 32%

2) Peak-to-valley gain factor at 1.15 keV
   - **ML (XGB)**: 1.80
   - Imaging $\lambda<1000$: 1.20

Preliminary
Summary

- **i-TED**: Imaging techniques to suppress the neutron induced background

- **Final i-TED 4pi** under development and MC simulations are key at this point
  - Optimization of the (n,g)/background discrimination capabilities
  - Realistic capture and background events

- **Results of (n,g)/background gain factor based on MC**
  - Coincidences + Analytical imaging cuts: i-TED gain factor 4-10 wrt C6D6
  - ML algorithms (XGB) promising: Similar background rejection + x2 (n,g) efficiency

- **ML background rejection with i-TED 5.3 data** (commissioning 2018 EAR1):
  - Training and tested with exp data (Au-197 and Fe-56) → Preliminary results
  - Background rejection equal or better than imaging cuts but
  - (n,g) efficiency 2-3 times larger
MC Simulation: background rejection

- MC study of capture/background discrimination
- Capture events: \textit{Au-197(n,g)} as a reference
  - Captugen + Geant4 PrimaryGenerator
- Neutron induced Background:
  - Full simulation: Time-cost + (probably) non-realistic
  - Experimental data measured @ EAR1 with i-TED 5.3: easy and realistic

\begin{itemize}
  \item CAPTUGEN Au-197(n,g)
  \item Geant4 Application i-TED 4pi
  \item Experimental background i-TED 5.3
  \item Output with same structure than exp data
  \item Capture/background discrimination
  \item Analytical Imaging cuts ML-algorithms
\end{itemize}
MC Results of (n,g)/background: i-TED gain with respect to C6D6

(n,g)/background gain BEFORE IMAGING

Scatterer alone similar to C6D6

Gain #1: Coincidences Absorber & Scatter

Gain #2: good CRT & only events with t1<t2

(under study)

Gain (n,g)/background wrt C6D6: x 1.5 - 3
MC Results of (n,g)/background: i-TED gain with respect to C6D6

- Scatterer alone similar to C6D6
- Gain #1: Coincidences Absorber & Scatter
- Gain #2: good CRT & only events with t1<t2 (under study)
- Gain (n,g)/background wrt C6D6: x 1.5 - 3

Why Background rejection with t1<t2?
MC Results of (n,g)/background: i-TED gain with respect to C6D6

**Why Background rejection with t1<t2?**

**Gain (n,g)/background wrt C6D6:** x 1.5 - 3

- **(n,g)/background gain BEFORE IMAGING**
  - Scatterer alone similar to C6D6
  - Gain #1: Coincidences Absorber & Scatter
  - Gain #2: good CRT & only events with t1<t2 (under study)

**Background event:**
- t1<t2

**Graph:**
- Scatterer
- Absorber
- Coincidences
- Coincidences & t1<t2
- C6D6 @ 100 mm

**Energy Diagram:**
- E1, r1, t1
- E2, r2, t2
- Background event: t1<t2
MC Results of \((n,g)/\text{background}\): i-TED gain with respect to C6D6

Why Background rejection with \(t_1 < t_2\)?

\((n,g)/\text{background}\) gain BEFORE IMAGING

- Scatterer alone similar to C6D6
- Gain #1: Coincidences Absorber & Scatter
- Gain #2: good CRT & only events with \(t_1 < t_2\) (under study)

Gain \((n,g)/\text{background}\) wrt C6D6: \(x 1.5 - 3\)
MC Results of \((n,g)/\text{background}\): i-TED gain with respect to C6D6

\((n,g)/\text{background}\) gain BEFORE IMAGING

- Scatterer alone similar to C6D6
- Gain #1: Coincidences Absorber & Scatter
- Gain #2: good CRT & only events with \(t_1 < t_2\)

Gain \((n,g)/\text{background}\) wrt C6D6: \(x \ 1.5 - 3\)

Why Background rejection with \(t_1 < t_2\)?

GOOD CRT RELEVANT
MC Results of \((n,g)/\text{background}\) gain with respect to C6D6

\(\text{(n,g)/background gain BEFORE IMAGING)\)
- Scatterer alone similar to C6D6
- Gain #1: Coincidences Absorber & Scatter
- Gain #2: good CRT & only events with \(t_1<t_2\)
  (under study)
- Gain \((n,g)/\text{background wrt C6D6}\) : x 1.5 - 3

\(\text{TOTAL (n,g)/background gain with IMAGING)\)
- i-TED gains a factor x 4 - 10 with respect to a C6D6 @ 10 cm
  depending of the sample - i-TED distance
  (Gain related to CRT not included)
ML-based (n,g)/bckg discrimination

- **Binary classifiers: different ML algorithms**
  - Logistic Regression: `from sklearn.linear_model import LogisticRegression`
  - Support Vector Classifier (SVC): `from sklearn.svm import SVC`
  - Gaussian Naive Bayes (NB): `from sklearn.naive_bayes import GaussianNB`
  - Random Forest: `from sklearn.ensemble import RandomForestClassifier`
  - **XGBoost Classifier**: `from xgboost import XGBClassifier`
  - Keras (neural network): `from tensorflow.keras.models import Sequential`

  **BEST ACCURACY + SIMPLICITY: XGB**
ML-based (n,g)/bckg discrimination

- ML-based capture/background discrimination in a nutshell

i-TED MC EVENTS: 9 variables!
Assign a binary flag

1 = CAPTURE
0 = BACKGROUND

MC + EXP EFFECTS
Energy, Time, Position resolution

TRAIN ML-ALGORITHM
BINARY CLASSIFIER
BALANCED N0 EVENTS

RESULT: CONFUSION MATRIX

(n,g) efficiency (fraction) = True positive

(n,g)/background gain factor = True positive/False Negative

TEST THE ML-ALGORITHM
(Remaining 20-30% MC events)
ML-based (n,g)/background discrimination: results XGB

IDEAL CRT (MC TIME):
BEST SCENARIO

DELTA_T NOT INCLUDED:
WORST SCENARIO

VERY PROMISING RESULTS:
- Background reduced to 26-37% of the original level
- Capture efficiency kept high: 63-74% of events
- Experimental situation between both results: Depends on CRT but also on the scatter-absorber and detector-sample distance
Imaging i-TED: (n,g) & background

**CAPTURE:** Reconstructed emission point for (n,g) events in the sample

Most of the reconstructed events concentrated around the sample position.

**BACKGROUND:** Reconstructed emission point for background from the walls

The distribution is much flatter with a broader maximum.
ML-algorithms vs imaging cut ($\lambda$)

**TAKE HOME MESSAGE:**
Background rejection based in MC events shows very promising results for ML-Algorithms

- High rejection of background
- Larger $(n,g)$ efficiency than imaging cuts

**MOTIVATES:**
Test ML-algorithms using exp. Data i-TED 5.3 (prototype commissioning (2018))
(V. Babiano’s talk for more details)
ML training: \((n,g)\) and background

**CAPTURE:** Au-197\((n,g)\)/Fe-56\((n,g)\)

**i-TED 5.3 @ EAR1**

**BACKGROUND:** Pb/C with i-TED 5.3 @ EAR1: Full spectrum

SAME ML ALGORITHM: **XGBoost** (Best performance in MC-based study)

Same training/testing procedure but replacing the MC input with exp. data
Results ML classifier: Au-197(n,g)

- ML (n,g)/background (n,g)/bckg discrimination applied to Au-197(n,g)

ML (XGB) training:
Au-197 (capture) + Pb (background)

Results of the ML-Classifier on Au-197(n,g)

1) Capture efficiency (4.9 eV res)
   ML (XGB): 80%
   Imaging λ<1000: 34%

1) Peak-to-valley gain factor
   ML (XGB): 1.24
   Imaging λ<1000: 1.14

Au-197: ML provides high (n,g) eff. but background is already low → Fe-56 better to check (n,g)/background gain
MC simulations i-TED 4π

- **Improved existing Geant4 application** for the response of the full i-TED:
  - Detailed geometry of i-TED 5 @ IFIC-lab
  - Simulation Read-out extended to four independent detectors

- **New simulation read-out** to include:
  - Flexible number of i-TED Modules: 1-4
  - Output: root file with same structure than experimental data (Same imaging codes!)
  - For each event: Egamma, E1, E2, r1,r2, t1, t2 , CoincidenceFlag

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i-TED 5 (each of the modules)
Background spectra for the MC simulations obtained from i-TED 5.3 @ EAR1

Different samples with large neutron scattering: very similar Edep spectra & TOF spectra → Spectrum has the same origin for all the samples

Studied the impact of i-TED intrinsic neutron sensitivity → Negligible!
Background spectra for the MC simulations obtained from \textit{i-TED 5.3 @ EAR1}.

Different samples with large neutron scattering: very similar Edep spectra & TOF spectra $\rightarrow$ Spectrum has the same origin for all the samples.

Studied the impact of i-TED intrinsic neutron sensitivity $\rightarrow$ Negligible!

**Conclusion:** Spectra representative of extrinsic background in EAR1.

GOAL: Obtain realistic Background due to scattered neutrons.
i-TED vs C6D6: (n,g) and activity

C6D6 @ 10 cm vs i-TED: (n,g) Efficiencies

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Au-197(n,g)</th>
<th>Pu-242(n,g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 keV</td>
<td>3.6%</td>
<td>4.5%</td>
</tr>
<tr>
<td>150 keV</td>
<td>3.1%</td>
<td>3.6%</td>
</tr>
<tr>
<td>250 keV</td>
<td>2.5%</td>
<td>2.7%</td>
</tr>
</tbody>
</table>

Geant4: efficiency 1x Bicron@100 mm:
- 3.1 - 3.5% (thr = 150 keV)
- 2.5 - 2.7% (thr = 250 keV)

Final efficiencies and activity rates for C6D6 and i-TED

Eff ratio C6D6/i-TED: Scatterer Singles ~ C6D6

C6D6/i-TED (n,g) 13.0
C6D6/i-TED activity C Rate 12.0
C6D6/i-TED @ 100 mm and i-TED @ 50 mm
C6D6/i-TED (n,g) 4
C6D6/i-TED activity C Rate 3.8
C6D6/i-TED activity w/ cuts 6.7

x13 if same distance
x4 if i-TED @ 50 mm
Results (n,g)/bckg discrimination
ML algorithms
ML-based \((n,g)/bckg\) discrimination

- **Binary classifiers: different ML algorithms**
  - **Logistic Regression**: `from sklearn.linear_model import LogisticRegression`
  - **Support Vector Classifier (SVC)**: `from sklearn.svm import SVC`
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**BEST ACCURACY + SIMPLICITY: XGB**
Extreme Gradient Boosting or XGBoost

• Supervised Machine-learning algorithm
• **Goal**: predict a target variable Y given a set of features – Xi.
• **How**: Combines several weak learners into a strong learner to provide a more accurate & generalizable ML model.
• **Multiple applications**: build a regression, **binary classification** or multi-class classification model.
• **Procedure**: Iterative technique known as boosting that builds a number of decision trees one after the other while focusing on accurately predicting those data points that were not accurately predicted in the previous tree.

### Example of parameter optimization

**BEST COMBINATION:**
- learning_rate = 0.1
- N_estimators = 150-200
ML bckg rejection

Random Forest

Naive Bayes

SVC

SVC + RBF kernel

Linear Regression

K-nearest neighbors

XGB (default)

XGB (120 trees, depth 8, subsample 0.7)
ML background rejection: XGB vs Keras

No delta T
WITH exp. Effects + THR
XGB: 63.13%
KERAS: 62.89%

WITH delta T,
WITH EXP. EFFECTS + THR
XGB: 73.98%
KERAS: 74.32%

v2) Removed 1 intermediate 50 neurons layer
Bckg rejection XGB: impact delta $\Delta T$

**NOW: Realistic resolutions**

- **200 ps: 70.98%**
  - XGB (Exp Effects + Thr)
  - Background: 0.7, Predicted: 0.3
  - Capture: 0.28, Predicted: 0.72

- **400 ps: 66.94%**
  - XGB (Exp Effects + Thr)
  - Background: 0.67, Predicted: 0.33
  - Capture: 0.33, Predicted: 0.67

- **600 ps: 65.10%**
  - XGB (Exp Effects + Thr)
  - Background: 0.65, Predicted: 0.35
  - Capture: 0.35, Predicted: 0.65

- **800 ps: 64.26%**
  - XGB (Exp Effects + Thr)
  - Background: 0.65, Predicted: 0.35
  - Capture: 0.36, Predicted: 0.64

- **1000 ps: 63.95%**
  - XGB (Exp Effects + Thr)
  - Background: 0.64, Predicted: 0.36
  - Capture: 0.36, Predicted: 0.64

- **1200 ps: 63.91%**
  - XGB (Exp Effects + Thr)
  - Background: 0.64, Predicted: 0.36
  - Capture: 0.37, Predicted: 0.63